

Test of a Jastrow-type wavefunction for a trapped few-body system in one dimension

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Abstract

For a system with interacting quantum mechanical particles in a one-dimensional harmonic oscillator, a trial wavefunction with simple structure based on the solution of the corresponding two-particle system is suggested and tested numerically. With the inclusion of a scaling parameter for the distance between particles, at least for the very small systems tested here the ansatz gives a very good estimate of the ground state energy, with the error being of the order of $\sim 1\%$ of the gap to the first excited state.

For a quantum many-body system with interacting particles, a trial wavefunction based on a product of functions for the motion of each individual pair was suggested some time ago by Jastrow [1] (who also referred to works by Mott, and Dingle [2]). This type of wavefunction forms the basis for many successful quantum Monte-Carlo methods (see e.g. Ref. [3]). In this study, a suggestion in Ref. [1] – to approximate the pair-motion function with the solution from a system with only two particles – is tested for a specific system, a one-dimensional harmonic oscillator with a few interacting quantum mechanical particles. One-dimensional quantum systems have been studied immensely, see e.g. Refs. [4–6] and references therein, though a majority of this research has focused on infinite systems. For confined systems with limited number of particles, various numerical approaches have been developed and used, see e.g. Refs. . The understanding of one-dimensional systems has become increasingly important with experimental developments such as ultra-cold atoms trapped in quasi-1D confinements [7], and electrons in carbon nanotubes [8] or semiconductor quantum wires [9]. For example, Ref. [10] reports about recent experiments on 1–10 ultracold atoms with tunable interactions, in a quasi-1D harmonic confinement.

The Hamiltonian considered here, expressed in dimensionless units, is

$$H = \sum_{i=1}^N \left(-\frac{1}{2} \frac{d^2}{dx_i^2} + \frac{1}{2} x_i^2 \right) + \sum_{i<j}^N V(x_i - x_j) \quad (1)$$

with the interaction V depending only on the relative distance between particles. For the ground state wave function, the ansatz considered here is of the form

$$\psi(x_1, \dots, x_N) \propto \left[\prod_{k=1}^N e^{-x_k^2/2} \right] \left[\prod_{i<j}^N f\left(\frac{x_i - x_j}{\sqrt{2}}\right) \right] \quad (2)$$

which can be shown to be exactly valid for a system with only two particles, in which case a coordinate transformation separates the Hamiltonian. As mentioned above, this type of wavefunction, based on the relative motion of pairs of particles rather than single-particle orbitals, was tried by Jastrow some time ago [1]. (Also note the similarity with equation (6) in Ref. [11]). For a system with only one spatial dimension one can ensure bosonic symmetry (or fermionic anti-symmetry) by choosing $f(x)$ as an even (or odd) function. For example, a system with non-interacting bosons (all in the lowest orbital) is then described with $f(x) = 1$. For fermions, setting $f(x) = x$ results in a Slater determinant with fermions in the N first orbitals (at least for small particle numbers this is straightforward to check).

This also implies that for bosons with an infinitely strong repulsive zero-range interaction, a so-called Tonks-Girardeau gas, the ground state is given by $f(x) = |x|$ [12, 13].

In this paper, the choice

$$f(x) = e^{+x^2/2}\phi(\alpha x)$$

is tested, where $\phi(x)$ is the relative wavefunction for the ground state of a system with just two particles, and α is a scaling factor. Such a scaling turns out to be necessary to get a reasonable energy. To be more precise, $\phi(x)$ is the solution corresponding to the lowest eigenvalue in the equation

$$\left(-\frac{1}{2}\frac{d^2}{dx^2} + \frac{x^2}{2} + V(\sqrt{2} \cdot x)\right)\phi(x) = E\phi(x)$$

where the factor of $\sqrt{2}$ is due to the coordinate transformation $x = (x_1 - x_2)/\sqrt{2}$ that is used to transform to the relative coordinate. For a general interaction V , $\phi(x)$ must be obtained by numerical means. This is here done with a diagonalization approach, with $\phi(x)$ expanded in harmonic oscillator orbitals (in the present study, 10–15 orbitals are used). The energy of the many-particle system is then evaluated (numerically) as $E = (\int \psi^* H \psi dx_1 \cdots dx_N) / (\int \psi^* \psi dx_1 \cdots dx_N)$. Unfortunately, because of computational limitations, the integration restricts this study to systems with only $N = 3$ particles. For comparison, the ground state energy obtained with a configuration interaction calculation (“exact diagonalization”) is used as reference.

For $N = 3$ particles, figure 1 shows how the energy depends on the scaling parameter α . An electrostatic Coulomb interaction with prefactor g is used, $V(x) = g/|x|$, regularized by assuming that the system is quasi-one-dimensional, with a tight harmonic confinement in the transverse directions (the transverse oscillator length is set to 10% of that in the axial direction). The figure shows results for different interaction strengths, and for both bosons and (spin-polarized) fermions. In all cases, the energy has a minimum around $\alpha = 0.9$. Based on the data at hand it is of course not possible to draw any general conclusions about e.g. the N -dependence in α .

For $g = 0.5$, the system is almost in a perturbative regime, where the ground state wavefunction is very similar to that of non-interacting particles. But for $g = 5$, the repulsion is so strong that the particles localize at individual positions (so called Wigner localization), demonstrated by those energies being very similar for both bosons and fermions. In either case, a wavefunction with the structure of equation 2 apparently can give a good approxi-

mation of the ground state. It is worth mentioning that the first excited state is one energy unit above the ground state, corresponding to an excited center-of-mass motion of the entire system. Since the energy of the trial wavefunction is close to the actual ground state, only a small fraction of the wavefunction can consist of states that are orthogonal to this.

To summarize, the results imply a simple recipe for how to get an approximative few-body wavefunction, given the two-body solution. While not intended as a practical approach for calculations, it does offer some intuitive insight in the structural properties of the ground state.

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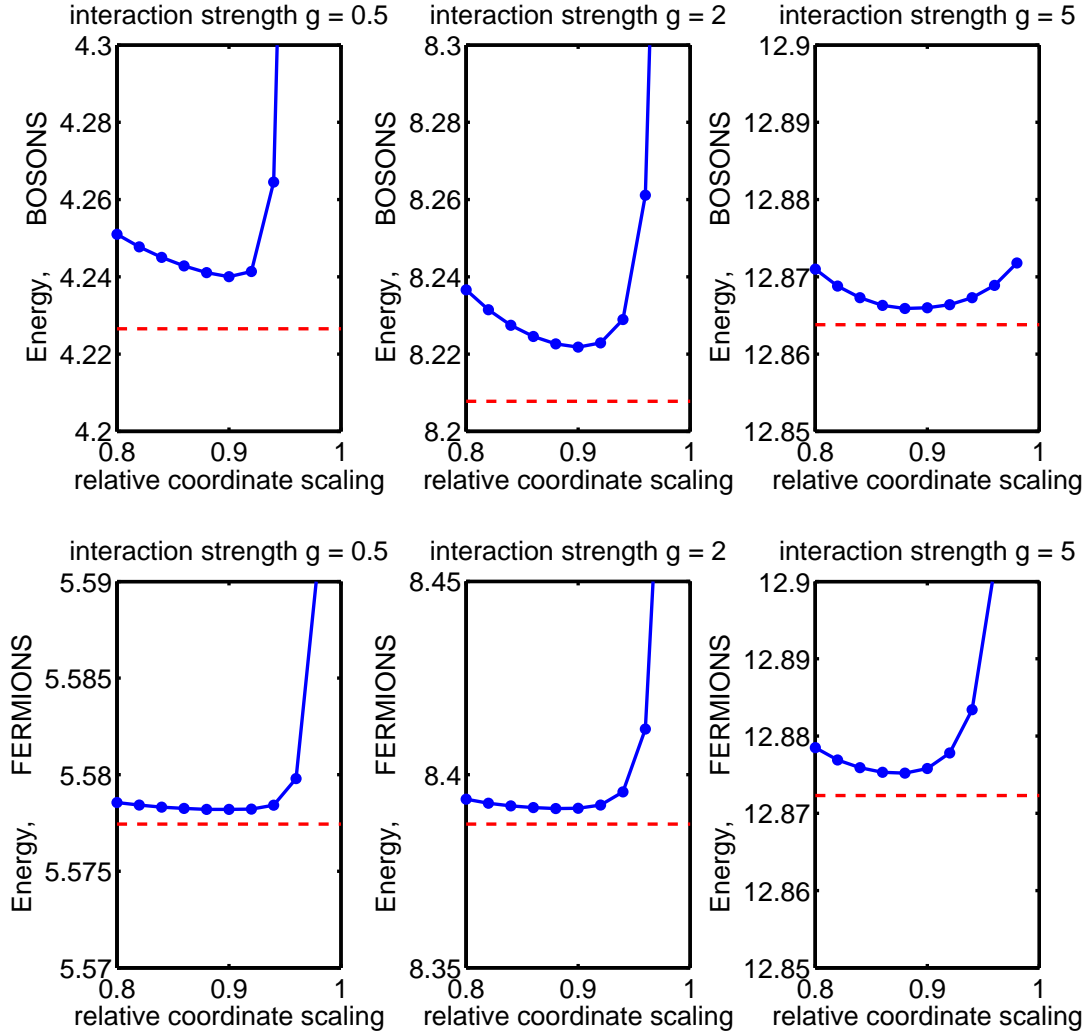


Figure 1: Results for $N = 3$ particles. The blue dots show the energy of the trial wavefunction as a function of the scaling parameter α . The dotted red lines show the energy from a configuration interaction calculation, included as reference. It should be noted that all values shown are still numerical approximations and only upper bounds. The reference energies are all converged in the calculation, and the errors estimated to be very small compared to the scale of the graphs. The energies obtained with the trial wavefunction also suffer from similar truncation errors, due to the linear expansion used for $\phi(x)$.